Atomic scale roughness of gold substrates

Solhjoo, Soheil; Vakis, Antonis I.

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Soheil Solhjoo and Antonis I. Vakis

Advanced Production Engineering (APE) — Engineering and Technology Institute Groningen (ENTEG)
Faculty of Mathematics & Natural sciences (FMNS) — University of Groningen (UG), the Netherlands

university of groningen

faculty of mathematics and natural sciences

ENTEG

Introduction

As a consequence of miniaturization of the mechanical devices, a large number of research studies are directed toward the tribological studies at the atomic scale, where the surface roughness plays a crucial role. Due to the limited lateral resolution of experimental devices in comparison to atomic spacing, researchers utilize atomistic computer simulation methods, such as classical molecular dynamics (MD), in order to investigate different processes, such as normal or frictional contacts. In these works, the substrate is represented, either, as a flat or a simple patterned surface; but, randomness does not vanish at the atomic scale.

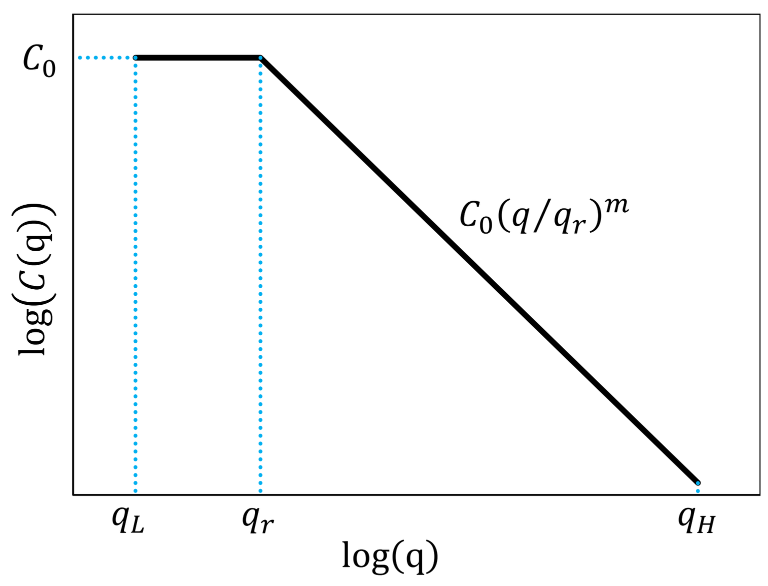
For treating such surfaces, different methods have been proposed in the literature: (1) generating a rigid custom-shaped substrate, or (2) generating a deformable substrate with an arbitrary surface profile. The stability of the initial substrate, however, has not yet been studied.

Goal: In this work, gold substrates with different surface roughness features were generated, and equilibrated. The surface roughness was analyzed due to this process, in order to propose a method for generating atomistic substrates with stable surface roughness features.

Rough Surfaces

Rough surfaces were described based on the following form of PSD

$$C(\mathbf{q}) = \begin{cases} C_0 & q_L \leq \|\mathbf{q}\| < q_r \\ C_0(\|\mathbf{q}\|/q_r)^m & q_r \leq \|\mathbf{q}\| \leq q_H \\ 0 & elsewhere \end{cases}$$



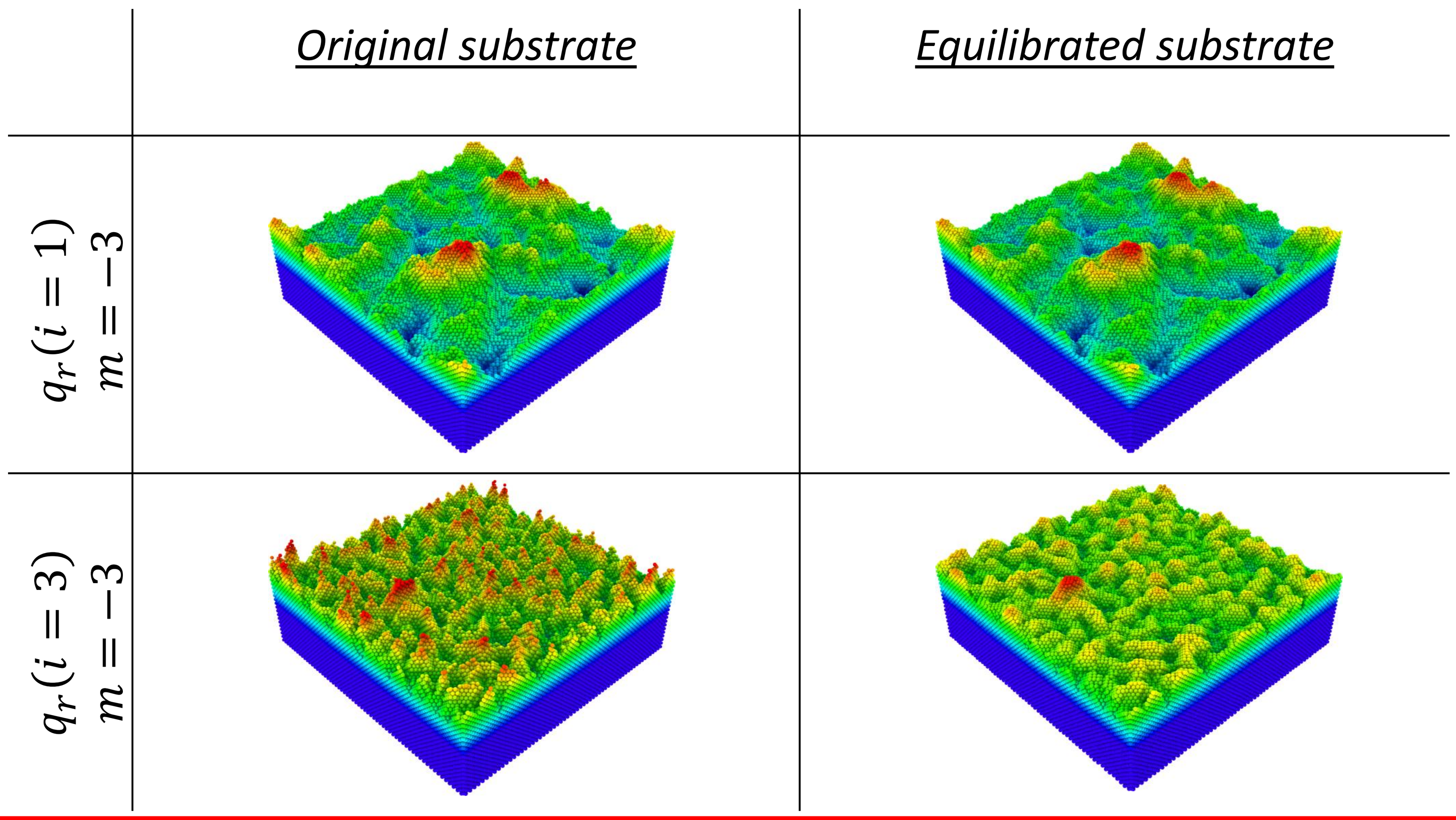
Conditions for generating the surfaces

Constants: $\begin{cases} q_L = \frac{2\pi}{L} = \frac{2\pi}{60a_0} \\ q_H = \frac{2\pi}{2a_0} \\ \sigma_{rms} = 2a_0 \end{cases}$, with $a_0 = 4.078$ Å

Variables: $\begin{cases} q_r(i) = q_L(q_H/q_L)^{i/4}, i \in [1,3] \\ m \in [-1,-5] \end{cases}$

Equilibration process

The surfaces were used to generate atomistic blocks. The rough substrates were equilibrated at 300 K for 1.5 ns.



A hybrid roughness parameter:

In order to analyze the surface roughness of the substrate a roughness parameter was defined as follows:

$$\rho = \frac{\zeta g}{\sigma_{rms}}, \text{with} \begin{cases} \zeta\text{: lateral correlation lentgh} \\ g\text{: RMS gradient} \end{cases}$$

$\rho = 0$ for a flat surface, and increases as the surface becomes rough.

Lateral Correlation Length:

It was found that the lateral correlation length has a minimum value of $\zeta_{min} \cong \sqrt{2}a_0 = \lambda_{min}/2$, where $\lambda_{min} = 2\sqrt{2}a_0$ is the shortest possible wavelength in an fcc structure.

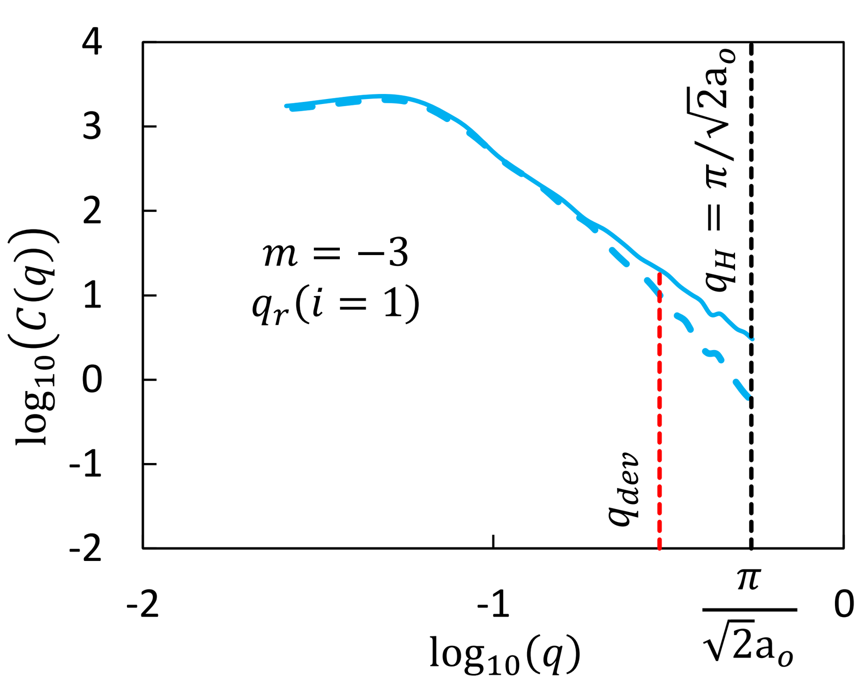
High frequency cutoff of PSD:

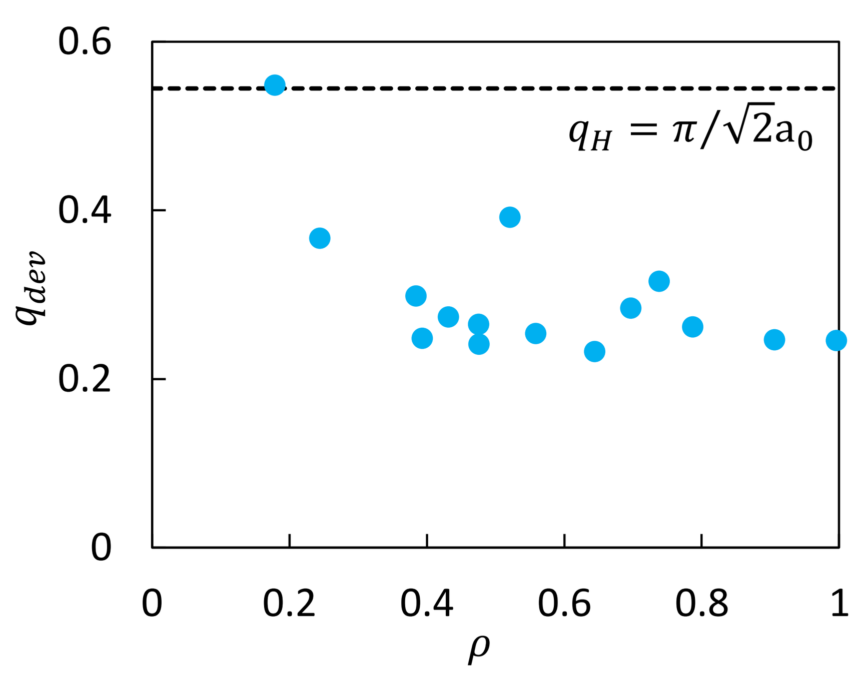
Based on the shortest possible wavelength in an fcc structure, the maximum wavenumber can be defined as $q_H = 2\pi/2\sqrt{2}a_0$.

Deviating wavenumber:

Comparing the changes of PSDs, a deviating wavenumber was defined as the wavenumber where $\left|\frac{C_{eq}-C_{in}}{C_{in}}\right| = 0.5$, where C_{in} and C_{eq} are the PSDs of the initial and equilibrated substrates, respectively.

- A higher value of q_{dev} indicates smaller changes due to equilibration.
- It was found that $q_{dev} \geq 0.2 \cong 2\pi/8a_0$.





Pseudo-stable atomistic rough substrates:

In order to generate an atomistic gold substrate with pseudo-stable roughness features, one of the following methods can be utilized.

1. Assuming $q_H \leq \max(q_{dev}) = 0.2$.

2. Constructing the rough surface using a three-segment PSD.

$$C(\mathbf{q}) = \begin{cases} C_0 & q_L \leq \|\mathbf{q}\| < q_r \\ C_0(\|\mathbf{q}\|/q_r)^{m_1} & q_r \leq \|\mathbf{q}\| \leq q_{dev} \\ C_1(\|\mathbf{q}\|/q_{dev})^{m_2} & q_{dev} \leq \|\mathbf{q}\| \leq q_H \\ 0 & elsewhere \end{cases}$$

- The results showed that: $\begin{cases} q_H \leq 2\pi/2\sqrt{2}a_0 \\ q_{dev} \leq 2\pi/8a_0 \\ m_2 \leq -4.5 \end{cases}$

References: **Simulations** were performed by LAMMPS [Plimpton (1995)], and **visualizations** were done by OVITO [Stukowski (2010)].